

4-Aminoazobenzene
60-09-3 | DTXSID6024460

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.49e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.99e-01

Confidence level: 5.25e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethylenediaminetetraacetic acid</div> <div>Measured: 1.40e-06</div> <div>Predicted: 2.81e-12</div>	<div>Image not found</div> <div>2-Phenyl-4,5-dichloro-3-pyridazinone</div> <div>Measured: 4.50e-07</div> <div>Predicted: 4.71e-05</div>	<div>Image not found</div> <div>Benzene, 1,4-bis(1-isocyanato-1-methylethyl)-</div> <div>Measured: 4.50e-07</div> <div>Predicted: 1.40e-03</div>
<div>Image not found</div> <div>alpha-Pinene oxide</div> <div>Measured: 2.31e-07</div> <div>Predicted: 8.58e-01</div>	<div>Image not found</div> <div>Benzene, 1,1'-ethenylidenebis-</div> <div>Measured: 4.91e-04</div> <div>Predicted: 1.69e-02</div>	